tomer

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FILE 'HOME' ENTERED AT 17:12:15 ON 13 JAN 2010

=> file casreact
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

FULL ESTIMATED COST

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FILE CONTENT: 1840 - 9 Jan 2010 VOL 152 ISS 3

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10599899a.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

TOh 13/01/2010

Structure attributes must be viewed using STN Express query preparation.

```
=> s 11 sss sam
SAMPLE SEARCH INITIATED 17:13:04 FILE 'CASREACT'
SCREENING COMPLETE -
                            O REACTIONS TO VERIFY FROM
                                                             0 DOCUMENTS
100.0% DONE
                  0 VERIFIED
                                  0 HIT RXNS
                                                                     0 DOCS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE
                                **COMPLETE**
                        BATCH
                                **COMPLETE**
PROJECTED VERIFICATIONS:
                                 0 TO
                                              0
PROJECTED ANSWERS:
                                 0 TO
                                              0
L2
              0 SEA SSS SAM L1 (
                                   0 REACTIONS)
=> s l1 sss full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 126.70 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 17:13:18 FILE 'CASREACT'
SCREENING COMPLETE -
                           63 REACTIONS TO VERIFY FROM
                                                              13 DOCUMENTS
100.0% DONE
                63 VERIFIED
                                   4 HIT RXNS
                                                                     1 DOCS
SEARCH TIME: 00.00.01
              1 SEA SSS FUL L1 (
L.3
                                   4 REACTIONS)
=> d 1-4
THE ESTIMATED COST FOR THIS REQUEST IS 3.14 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) / N: y
T.3
     ANSWER 1 OF 1 CASREACT COPYRIGHT 2010 ACS on STN
RX(15) OF 21 - 2 STEPS
                     1.1. C:9024-90-2,
                          Water
                     1.2. H3PO4, Water
                                                      NH_2
           ÇN
                     1.3. KOH, Water
                     2.1. Ni, Me2CHOH, KOH,
   NC-CH2-CH-Bu-i
                                                         CO<sub>2</sub>H
                          H2, Water
                                              i-Bu
                     2.2. AcOH
                     2.3. KOH, Water
                     2.4. AcOH, Me2CHOH
REF: PCT Int. Appl., 2005100580, 27 Oct 2005
NOTE: 1) biotransformation, enzymic, stereoselective, NIT-102 C2 used,
      buffered soln., 2) Raney nickel used, alternative preparation
      shown
      STEP(1.1) 24 hours, 30 deg C; 24 hours, 30 deg C; 24 hours,
CON:
          30 deg C; 24 hours, 30 deg C
      STEP(1.2) pH 2.1
      STEP(2.1) overnight, room temperature, 50 psi
      STEP(2.2) room temperature -> 50 deg C, acidify; 50 deg C;
```

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STEP(2.4) overnight, room temperature, acidify

overnight, room temperature STEP(2.3) pH >7

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